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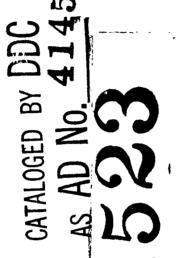CAMERON STATION, ALEXANDRIA, VIRGINIA

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MEMORANDUM
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AUGUST 1963

INVARIANT IMBEDDING
AND THE ANALYSIS OF PROCESSES

Robert Kalaba

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SANTA MONICA • CALIFORNIA

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PREFACE

One of the most characteristic features of systems is that they undergo processes. Hence, general systems theory must concern itself with the theory of processes. It is clear that a given physical process can be described mathematically in intrinsically different ways, each having advantages and disadvantages.

The aim of this Memorandum is to describe the invariant imbedding approach to the study of processes, an approach which enables us to convert boundary value problems into initial value problems. This is a great computational advantage and is frequently of use analytically. There are immediate applications in mathematical physics and in the modern theory of automatic control, where two-point boundary value problems for Euler equations abound. The Memorandum should be of interest to mathematical physicists, control engineers, and operations analysts.

SUMMARY

Many of the processes considered in modern physics and control theory lead, from the mathematical viewpoint, to nonlinear two-point boundary-value problems. These problems are difficult to treat computationally and analytically. A goal of the theory of invariant imbedding is to provide a systematic technique for converting these boundary-value problems into initial-value problems through use of appropriate variables and the employment of functional equation techniques.

A particle multiplication process is considered for illustrative purposes. The classical equations and the invariant imbedding equations are derived and various interconnections are discussed. The paper is intended to be self-contained.

vii

CONTENTS

I. INTRODUCTION

One of the most important features of systems is that they undergo processes. Thus it is that a general theory of systems must concern itself with the theory of processes. The aim of this paper is to provide an introduction to some recent developments in the theory of processes.

Customarily when studying a particular process, we focus our attention on it and attempt to discern those properties which are of interest to us. For example, we may describe the state of a system S by means of a vector p, which is viewed as a point in a phase space. The local properties of the process are given by specifying that a system in a state p at time n will be in state q at time n + 1. This is symbolized by writing

$$(1) \qquad q = T(p,n).$$

Here we are assuming that the process is deterministic and that cause and effect are known. If the initial state is c and if the state at time n is p_n, then the process is described by the equations

$$(2) \qquad p_0 = c,$$

$$(3) \qquad p_{n+1} = T(p_n,n), \quad n = 0,1,2,\ldots.$$

We might, for example, wish to determine whether the system remains in a certain region of phase space over all time or not.

One of the key conceptual tools for studying such processes, which are viewed as sequences of transformations of the state of

the system, is the observation that the state at time n is a function of the initial state c and the time n, i.e.,

$$(4) \qquad p_n = f(c,n).$$

Furthermore this function $f(c,n)$ has a semi-group [1] property expressed by the equation

$$(5) \qquad f(c,m + n) = f(f(c,n),m).$$

This is a symbolic representation of the fact that the state at time $m + n$, the initial state having been c, can be viewed as having been attained by letting n units of time pass, so that the system is transformed into the state $f(c,n)$, and then, considering this as a new initial state, letting an additional m units of time pass. Notice that use of this principle leads us to consider not only the single process of duration $m + n$ and initial condition c, but a class of processes of arbitrary duration and arbitrary initial condition.

In essence, invariant imbedding is a generalization of this concept. To study a particular process we imbed that process in an appropriate class of processes. Then we express the relationships among the properties of the members of the class. These relations then constitute an analytical description of the processes. In this way we are frequently able to forge new tools for their analytic and computational study. As a rule this leads to the employment of other variables such as length or energy, in addition to the classical one, time, as the semi-group variable.

A discussion of the mathematical treatment of processes, including stochastic, adaptive, and control aspects can be found in [2]. A discussion of invariant imbedding with applications to neutron transport theory, multiple scattering, diffusion, etc., is given in [3] where references to the work of Ueno, Redheffer, Preisendorfer and others will be found. Basic references to the pioneering efforts of S. Chandrasekhar can be found in [4]. Our aim is to show how boundary-value problems can be transformed into initial-value problems, a desire prompted in part by the desire to make it easier to bring the power of modern digital computers to bear in significant classes of problems.

In subsequent sections we shall illustrate these general remarks by considering a particle multiplication process. The physical background is provided, the standard description of the process is presented, and then the treatment via invariant imbedding is indicated. Various interconnections are discussed, and some computational and analytical aspects are illuminated. There are immediate applications to analytical dynamics and automatic control theory. The discussion is intended to be self-contained.

II.   THE CLASSICAL TRANSPORT EQUATIONS [3]

Let us consider a particle process which takes place within a thin tube. The tube, assumed homogeneous, extends along a t-axis from $t = 0$ to $t = T$. At the right end, $t = T$, a steady stream of c particles per unit time is incident on the tube and at the end $t = 0$ a stream of w particles per unit time is incident on the tube. Within the rod the particles interact with one another and with the material of which the rod is constructed. The flows within the tube are described by the functions $u(t)$ and $v(t)$, where

(6) $u(t)$ = the number of particles per second passing
                        the point t and traveling to the right,

and

(7) $v(t)$ = the number of particles per second passing
                        the point t and traveling to the left,

(8) $0 \leq t \leq T.$

The interactions which take place are described by assuming that when a flow u to the right and a flow v to the left are incident on a section of tube of length Δ, the increment in the flow to the right is $F(u,v)\Delta + o(\Delta)$, and the increment in the flow to the left is $G(u,v)\Delta + o(\Delta)$. Consequently, we may write the equations

(9) $u(t + \Delta) - u(t) = F(u(t),v(t))\Delta + o(\Delta),$

(10) $v(t) - v(t + \Delta) = G(u(t),v(t))\Delta + o(\Delta),$

where, as usual, $o(\Delta)$ is a function of Δ having the property that

$$(11) \qquad \lim_{\Delta \to 0} \frac{o(\Delta)}{\Delta} = 0.$$

Upon dividing Eqs. (9) and (10) by Δ and letting Δ tend to zero, we find the relations

$$(12) \qquad \frac{du}{dt} = F(u,v),$$

$$(13) \qquad -\frac{dv}{dt} = G(u,v).$$

Furthermore, in view of the assumptions made concerning the flows which are incident on the tube, we have the boundary conditions

$$(14) \qquad v(T) = c,$$

$$(15) \qquad u(0) = w.$$

In this manner we are led, along classical lines, to study the two-point boundary-value problem of Eqs. (12) - (15). Nonlinear two-point boundary-value problems are known to be quite intractable, both analytically and computationally [5].

III. THE REFLECTION AND TRANSMISSION FUNCTIONS [6]

To apply the idea of invariant imbedding to the particle

process discussed earlier, we consider the class of processes

taking place in identical homogeneous tubes of lengths $T \geq 0$,

subject to incident fluxes, at the right end, of $c \geq 0$. The flux

incident on the left end is held fixed at a particular value, w.

The physical situation suggests that we consider the fluxes which

emerge from the right and left ends of the various tubes, which

we call the "reflected" and the "transmitted" fluxes. Note that

the reflected flux which emerges from the tube of length T, due

to an incident flux c on the right end, is a function of c and T.

Since there is a constant flux w which is incident on the left

ends of the tubes, it is true that the fluxes which emerge from

the tube are dependent on w, but we suppress this dependence since

it plays no real role in our considerations. The reflected flux

is denoted by

$$(16) \qquad r = r(c,T).$$

Similarly, we denote the transmitted flux by

$$(17) \qquad \tau = \tau(c,T).$$

First we observe that the fluxes which emerge from a rod of

zero length are known, namely,

$$(18) \qquad r(c,0) = w,$$

(19) $\tau(c,0) = c.$

Next we set about relating the transmitted and reflected fluxes for rods of neighboring lengths; more precisely, we express the flux reflected from rods of length $T + \Delta$ in terms of the flux reflected from rods of length T. Our basic relation is

(20) $r(c,T + \Delta) = r(c + G(r,c)\Delta,T) + F(r,c)\Delta + o(\Delta).$

This equation expresses the fact that the flux reflected from a rod of length $T + \Delta$, due to an incident flux c, consists of three parts:

A. Flux which is reflected from a rod of length T due to an input flux c which is modified by passage through a section of length Δ, and so is of strength $c + G(r,c)\Delta + o(\Delta)$.

B. An increment in the flux to the right due to incident fluxes of strengths r and c on a tube of length Δ.

C. Fluxes which are proportional to the second and higher powers of Δ.

Upon letting Δ tend to zero in Eq. (20), we arrive at the desired equation

(21) $r_T = G(r,c)r_c + F(r,c),$

where the subscripts denote partial derivatives.

In general Eq. (21) is a first-order nonlinear partial differential equation. Since it is linear in the partial derivatives r_T and r_c, it is referred to as a quasilinear partial differential equation [7]. It is to be solved for the reflection function

(22) $r = r(c,T),$

subject to the initial condition in Eq. (3).

In a similar manner we see that the transmission function $\tau(c,T)$ satisfies the relation

(23) $\tau(c,T + \Delta) = \tau(c + G(r,c)\Delta,T) + o(\Delta).$

In the limit, as Δ tends to zero, this becomes

(24) $\tau_T = G(r,c)\tau_c.$

In addition, the transmission function $\tau = \tau(c,T)$ is subject to the initial condition in Eq. (19).

Thus we have succeeded in relating the reflection and transmission properties of tubes of neighboring lengths and incident fluxes to each other. In addition, the transmission and reflection properties of a tube of zero length are known. In this manner we may determine the functions $r(c,T)$ and $\tau(c,T)$ computationally for a desired set of values of the variables c and T.

IV. DETERMINATION OF THE INTERNAL FLUXES IN TERMS
OF THE REFLECTED AND TRANSMITTED FLUXES

First let us note that if the function $r(c,T)$ is known, then the boundary-value problem posed earlier is, in effect, transformed into an initial-value problem. For at the right end of the rod both the flux traveling to the left

$$(25) \qquad v(T) = c$$

and the flux traveling to the right

$$(26) \qquad u(T) = r(c,T)$$

are known. However, even more may be said.

Consider an interior point t, where the two fluxes are $u(t)$ and $v(t)$. We may consider that a flux $v(t)$ is incident on a rod of length t, giving rise to a reflected flux $u(t)$; i.e.,

$$(27) \qquad u(t) = r(v(t),t).$$

Furthermore, making use of the transmission function, we note that under these conditions the flux emerging from the left end of the tube, $v(0) = b$, is

$$(28) \qquad b = \tau(v(t),t).$$

If now the Eqs. (27) and (28) are solved for u and v in terms of t, b, and w, then we shall have obtained a general solution of the original system of nonlinear differential equations. Though these observations are evident on physical grounds, we can easily verify

that if $u(t)$ and $v(t)$ are two functions that satisfy the relations
(27) and (28), where $r(c,T)$ and $\tau(c,T)$ are the reflection and trans-
mission functions which satisfy Eqs. (21) and (24), then the func-
tions $u(t)$ and $v(t)$ satisfy the original nonlinear transport equa-
tions. In more picturesque language, we may say that a knowledge
of the reflection and transmission functions enables us to determine
the fluxes within the tube.

Differentiation of Eq. (28) with respect to t yields the
relation

$$(29) \qquad 0 = \tau_v \frac{dv}{dt} + \tau_t.$$

Upon comparison with Eq. (24) we see that

$$(30) \qquad -\frac{dv}{dt} = G(u,v),$$

providing that

$$(31) \qquad \tau_v \neq 0.$$

Next we differentiate Eq. (27) with respect to t which yields

$$(32) \qquad \frac{du}{dt} = r_v \frac{dv}{dt} + r_t$$

$$= - r_v G + r_t.$$

Comparison with Eq. (21) then shows that

$$(33) \qquad \frac{du}{dt} = F(u,v).$$

Thus our assertion is established.

Let us note that the assumption

$$(34) \qquad \tau_v \neq 0$$

is a reasonable one, stating that the transmitted flux is not independent of the incident flux. Furthermore the constants b and w have the physical interpretations

$$(35) \qquad u(0) = r(v(0),0) = w,$$

$$(36) \qquad b = \tau(v(0),0) = v(0).$$

V. AN ILLUSTRATIVE EXAMPLE

As an illustration consider a neutron multiplication process in which a particle traversing a section of a homogeneous tube of length h has a probability of $ah + o(h)$ of being absorbed by the medium. Upon absorption the original particle disappears and is replaced by two daughter particles, one traveling in each direction. The tube is of length T and a flux of average strength c is incident on the right end of the tube and no flux is incident on the left end. In this case it is easy to see that the equations for the average internal fluxes are [8]

$$(37) \qquad u(t + h) = u(t) + ahv(t) + o(h),$$

$$(38) \qquad v(t) = v(t + h) + ahu(t) + o(h),$$

which become, upon letting h tend to zero,

$$(39) \qquad \frac{du}{dt} = av,$$

$$(40) \qquad -\frac{dv}{dt} = au.$$

The boundary conditions are

$$(41) \qquad u(0) = 0, \quad v(T) = c.$$

Since

$$(42) \qquad F(u,v) = av$$

and

$$(43) \qquad G(u,v) = au,$$

the equations for the reflected and transmitted fluxes are

$$(44) \qquad r_T = ac + arr_c$$

and

$$(45) \qquad \tau_T = ar\tau_c.$$

In view of the linearity of Eqs. (39) and (40), and on physical grounds, we expect that the reflected flux will be proportional to the incident flux c,

$$(46) \qquad r(c,T) = R(T)c.$$

If we substitute this expression into Eq. (44), we find

$$(47) \qquad \frac{dR}{dT} c = ac + aR^2c,$$

or

$$(48) \qquad \frac{dR}{dT} = a(1 + R^2),$$

an ordinary differential equation for the reflection coefficient $R(T)$. For an initial condition we have

$$(49) \qquad R(0) = 0.$$

The function $R(T)$ can be found explicitly and is

$$(50) \qquad R(T) = \tan a \, T.$$

Thus for the reflection function $r(c,T)$ we have

$$(51) \qquad r(c,T) = c \tan aT.$$

This is an interesting formula in itself and shows that if the length

of the tube is sufficiently great, $\pi/(2a)$ to be exact, then the reflected flux becomes infinite. Thus the "critical length" of the tube is

$$(52) \qquad T_{crit} = \frac{\pi}{2a} .$$

In a similar manner we find that

$$(53) \qquad \tau(c,T) = c \sec aT.$$

To find the internal fluxes we use the integration theory sketched above. First we write

$$(54) \qquad u = v \tan at,$$

$$(55) \qquad b = v \sec at.$$

Upon solving for u and v we find

$$(56) \qquad v(t) = b \cos at,$$

$$(57) \qquad u(t) = b \sin at,$$

the solutions of Eqs. (39), (40), and (41).

VI. RIGOROUS DERIVATION OF THE EQUATIONS FOR THE REFLECTED AND TRANSMITTED FLUXES [9]

In earlier sections we showed how to deduce the equations for the reflected and transmitted fluxes using a physical argument. It is important, though, to have a purely mathematical procedure. In fact, as I. Busbridge points out in her book [10], "The application of these (invariance) principles is not easy and until a precise statement is given of the physical conditions which are sufficient to ensure their truth, any solution based on these ought to be verified in another way." In this section we shall show how to deduce the equations for the reflected and transmitted fluxes from the equations for the internal fluxes in a purely mathematical manner. We shall see that the essential feature is the uniqueness of the solution of the linear perturbation equations of the internal flux equations. The basic idea behind the discussion is that there is essentially only one set of perturbation equations, regardless of what is varied.

Let us consider the equations

$$(58) \qquad \frac{du}{dt} = F(u,v), \quad u(0) = 0,$$

$$(59) \qquad -\frac{dv}{dt} = G(u,v), \quad v(T) = c.$$

In addition we consider the same equations for the functions $U(t)$ and $V(t)$ on the interval $t = 0$ to $t = T + h$, with the same boundary conditions,

$$(60) \qquad \frac{dU}{dt} = F(U,V), \quad U(0) = 0,$$

$$(61) \qquad -\frac{dV}{dt} = G(U,V), \quad V(T + h) = c.$$

We may refer these equations to the interval $t = 0$ to $t = T$ by noting that

$$(62) \qquad V(T) = c - V'(T)h = c + G(U(T),V(T))h$$
$$= c + G(u(T),v(T))h.$$

In the above equations we have suppressed all terms involving powers of h higher than the first. For ease in writing we shall continue to do this throughout the section. Next we introduce the perturbation functions $w(t)$ and $x(t)$ via the relations

$$(63) \qquad U(t) = u(t) + w(t)h,$$

$$(64) \qquad V(t) = v(t) + x(t)h,$$

which hold for $0 \leq t \leq T$.

If we write

$$(65) \qquad U(T + h) = U(T) + U'(T)h$$
$$= u(T) + w(T)h + F(u(T),v(T))h$$

and

$$(66) \qquad V(0) = v(0) \div x(0)h,$$

we see that we must study $w(T)$ and $x(0)$ in more detail.

We know that the functions $w(t)$ and $x(t)$ satisfy the linear perturbation equations

$$(67) \qquad \frac{dw}{dt} = F_u(u,v)w + F_v(u,v)x,$$

$$(68) \qquad -\frac{dx}{dt} = G_u(u,v)w + G_v(u,v)x.$$

As boundary conditions we have

$$(69) \qquad w(0) = 0$$

and

$$(70) \qquad x(T) = G(u(T),v(T)).$$

The second condition follows from Eq. (62). In addition, we see that if we regard the functions $u(t)$ and $v(t)$ as functions of the parameter c, then

$$(71) \qquad \frac{d}{dt} u_c = F_u(u,v)u_c + F_v(u,v)v_c,$$

$$(72) \qquad -\frac{d}{dt} v_c = G_u(u,v)u_c + G_v(u,v)v_c.$$

Furthermore the functions u_c and v_c satisfy the boundary conditions

$$(73) \qquad u_c(0) = 0,$$

$$(74) \qquad v_c(T) = 1.$$

If we now assume that there is a unique solution of Eqs. (67) and (68), subject to the conditions (69) and (70) on the interval $[0,T]$, then we have the desired results

$$(75) \qquad w = G(u(T),v(T))u_c$$

and

$$(76) \qquad x = G(u(T),v(T))v_c.$$

For T sufficiently small this assumption is certainly justified.

Equation (65) now becomes

$$(77) \qquad U(T + h) = u(T) + u_c G(u(T),v(T))h + F(u(T),v(T))h.$$

Upon writing

$$(78) \qquad u(T) = r(c,T),$$

and letting h tend to zero, we find

$$(79) \qquad \frac{\partial r}{\partial T} = G(r,c) \frac{\partial r}{\partial c} + F(r,c).$$

This is the desired equation for the reflection function. Equation (66) becomes

$$(80) \qquad V(0) = v(0) + G(u,(T),v(T))v_c h]_{t=0}.$$

This leads to our equation for the transmission function

$$(81) \qquad \frac{\partial r}{\partial T} = G(r,c) \frac{\partial T}{\partial c}.$$

In the above manner we see how the mathematical relations between the equations for the transmitted and reflected fluxes and those for the internal fluxes arise. These relationships may be illuminated from a different mathematical viewpoint as is shown in [11]. There, for linear systems, it is shown that the equations for the internal fluxes can be considered as arising as Euler equations for a certain quadratic variational problem. The equations

for the reflected and transmitted fluxes arise upon applying the
principle of optimality [5] to the same quadratic variational
problem. Lastly, let us note that results of the foregoing nature
contain the variational formulas for one-dimensional Green's func-
tions and for the characteristic functions and characteristic
values [12]. The same method applies to time-dependent and other
transport processes.

VII. DISCUSSION

A given physical process can be considered from various
mathematical viewpoints. It is to be expected that certain prop-
erties will be more apparent from some viewpoints than from others.
Frequently the classical derivations lead to boundary-value problems
which are difficult to treat, especially from the computational
viewpoint. One way of overcoming these difficulties is through use
of the functional equation techniques of invariant imbedding, as
we have seen.

Many of the classical equations of mathematical physics [7]
as well as those of modern automatic control theory [13] arise in
the form of Euler equations associated with the minimization of
certain functionals. As a rule boundary conditions either are given
or arise in the form of free boundary conditions. Thus it is that
a major problem in all of modern physics and control theory is the
resolution of boundary-value problems. Application of invariant
imbedding to dynamics can be found in [14,15]. An alternative to
the usual Hamilton-Jacobi theory is provided.

The considerations of this paper are readily generalized to
systems of equations of order higher than two [6]. They are also
applicable to the differential-integral equations which arise in
neutron transport theory [16] and radiative transfer [17].

From the conceptual viewpoint let us point out that the
establishing of existence and uniqueness of solution for nonlinear
two-point boundary-value problems is difficult. Invariant imbedding

offers one avenue of approach [18]. The close conceptual relation
between invariant imbedding and dynamic programming is evident [5].

Finally let us note that a direct computational attack on
nonlinear two-point boundary-value problems is possible via quasi-
linearization [19].

REFERENCES

1. Hille, E., and R. Phillips, _Functional Analysis and Semi-Groups_, American Mathematical Society, Providence, R. I., 1957.

2. Bellman, R., and R. Kalaba, "Dynamic Programming and Adaptive Processes," _IRE Trans. on Automatic Control_, Vol. AC-5, 1960, pp. 5-10.

3. Bellman, R., R. Kalaba, and G. M. Wing, "Invariant Imbedding and Mathematical Physics--I: Particle Processes," _J. Math. Phys._, Vol. 1, 1960, pp. 280-308.

4. Chandrasekhar, S., _Radiative Transfer_, Dover Publications, Inc., New York, N. Y., 1960.

5. Bellman, R., _Adaptive Control Processes: A Guided Tour_, Princeton University Press, Princeton, N. J., 1961.

6. Bellman, R., R. Kalaba, and G. M. Wing, "Invariant Imbedding and the Reduction of Two-point Boundary-value Problems to Initial-value Problems," _Proc. Nat. Acad. Sci. USA_, Vol. 46, 1960, pp. 1646-1649.

7. Courant, R., and D. Hilbert, _Methods of Mathematical Physics_, Vol. 2, Interscience Publishers, New York, N. Y., 1962.

8. Bellman, R., and R. Kalaba, "Transport Theory and Invariant Imbedding," a chapter in the book _Nuclear Reactor Theory_, American Mathematical Society, Providence, R. I., 1961.

9. Bellman, R., and R. Kalaba, "On the Fundamental Equations of Invariant Imbedding," _Proc. Nat. Acad. Sci. USA_, Vol. 47, 1961, pp. 336-338.

10. Busbridge, I., _The Mathematics of Radiative Transfer_, Cambridge University Press, London, 1960.

11. Bellman, R., R. Kalaba, and G. M. Wing, "Invariant Imbedding and Variational Principles in Transport Theory," _Bull. Amer. Math. Soc._, Vol. 67, 1961, pp. 396-399.

12. Bellman, R., and R. S. Lehman, "Functional Equations in the Theory of Dynamic Programming--X: Resolvents, Characteristic Functions and Values," _Duke Math. Journal_, Vol. 27, 1960, pp. 55-70.

13. Pontryagin, L., et al., _The Mathematical Theory of Optimal Processes_, Interscience Publishers, New York, N. Y., 1962.

14. Bellman, R., and R. Kalaba, "A Note on Hamilton's Equations and Invariant Imbedding," Quart. of Appl. Math., to appear.

15. Bellman, R., and R. Kalaba, Invariant Imbedding and the Integration of Hamilton's Equations, The RAND Corporation, RM-3538-PR, February 1963.

16. Wing, G. M., An Introduction to Transport Theory, John Wiley and Sons, Inc., New York, N. Y., 1962.

17. Bellman, R., R. Kalaba, and M. Prestrud, Invariant Imbedding and Radiative Transfer in Slabs of Finite Thickness, Elsevier Publishing Co., New York, N. Y., 1963.

18. Bellman, R., R. Kalaba, and G. M. Wing, "Dissipation Functions and Invariant Imbedding, I," Proc. Nat. Acad. Sci. USA, Vol. 46, 1960, pp. 1145-1147.

19. Kalaba, R., "On Nonlinear Differential Equations, the Maximum Operation and Monotone Convergence," J. of Math. and Mech., Vol. 8, 1959, pp. 519-574.